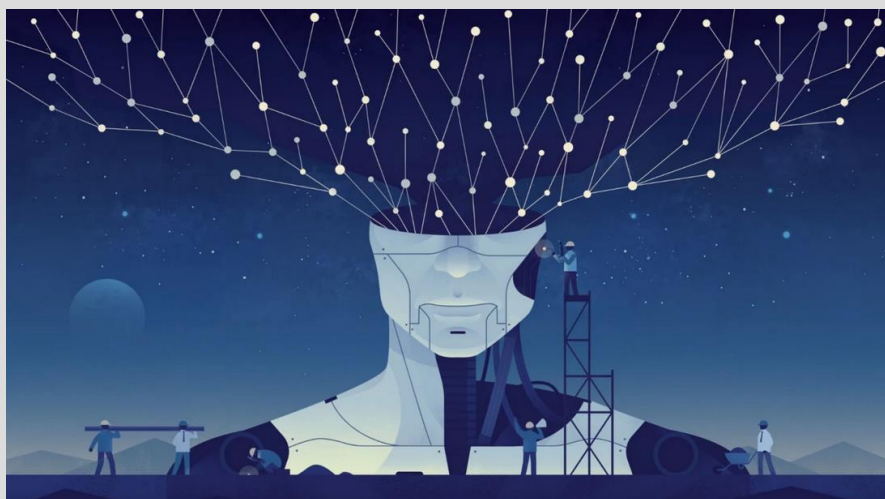


# Background neural networks tutorial

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20-03-2020



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Institute for Molecular Life Sciences  
**Radboudumc**

# Teaching goals

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1. Basic understanding of neural networks
2. Get familiar with terms
3. Get some hand on experience (2<sup>nd</sup> presentation)

# Content

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- Software
- Building blocks
  - Neurons
  - Loss functions
  - Back propagation
- Practicalities
- Architectures
- Problems / questions

# Software

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- **Software**
- Building blocks
  - Neurons
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# Software

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- TensorFlow
- Keras
- **Pytorch**



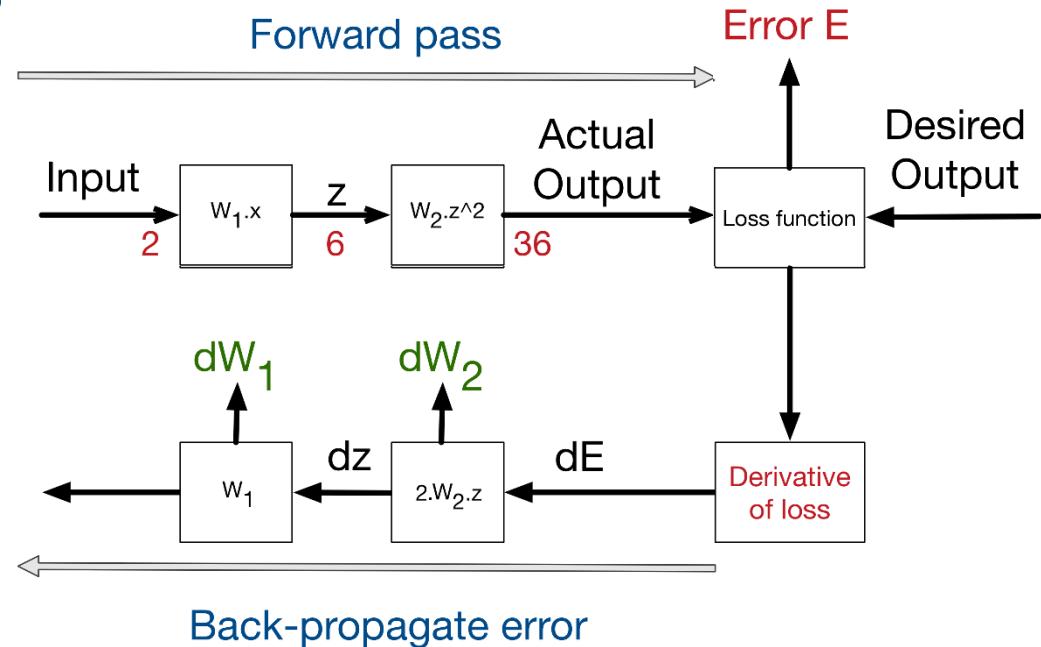
# Building blocks

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- Software
- **Building blocks**
  - Neurons
  - Loss functions
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# Building blocks

- Neurons / networks
- Loss function
- Back propagation



# Recap: vectors

- Row times column
- Vectors to matrix

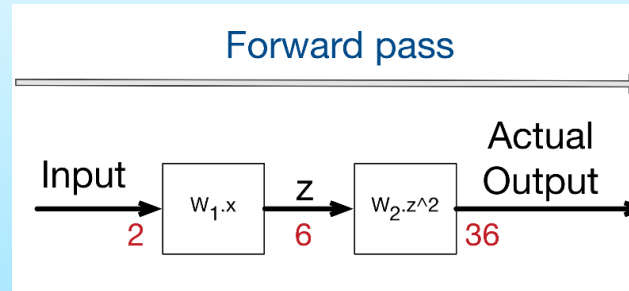
$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \cdot \begin{bmatrix} b_{11} \\ b_{21} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} \\ a_{21}b_{11} + a_{22}b_{21} \end{bmatrix}$$

$$\begin{bmatrix} 2 \\ 3 \\ 4 \end{bmatrix} \times \begin{bmatrix} 6 & 4 & 3 \end{bmatrix} = \begin{bmatrix} 12 & 8 & 6 \\ 18 & 12 & 9 \\ 24 & 16 & 12 \end{bmatrix}$$



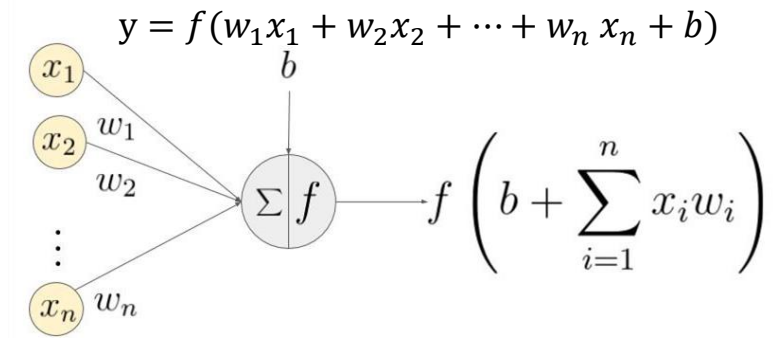
# Building blocks

- Software
- Building blocks
  - **Neurons**
  - Loss functions
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- Problems / questions



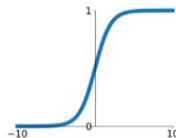
# Building block: neuron

- Data transformer: input  $\rightarrow$  output
  - Activation function (Input \* Weight + Bias)
- Vectors  $\rightarrow Y = f(X \cdot W + b)$
- Non-linear



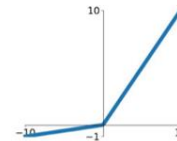
## Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



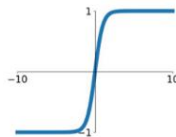
## Leaky ReLU

$$\max(0.1x, x)$$



## tanh

$$\tanh(x)$$

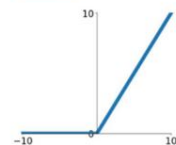


## Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

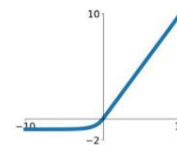
## ReLU

$$\max(0, x)$$



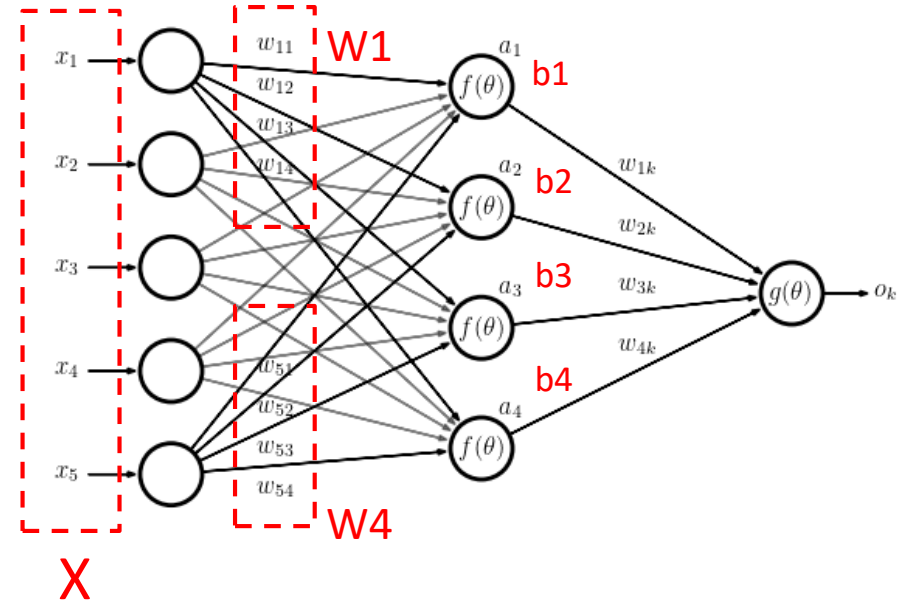
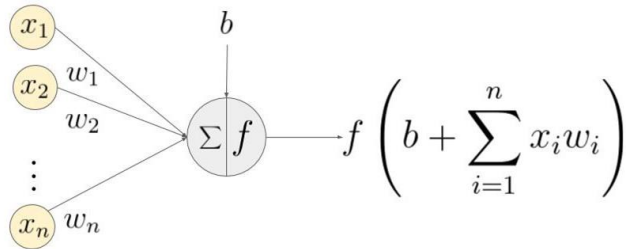
## ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



# Building block: Neural Network

- Network of neurons



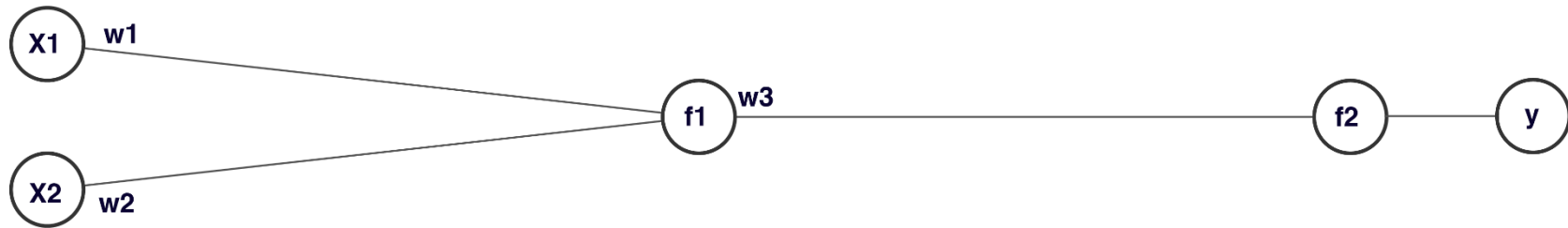
# Neural Network – example1

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$$y = f_2( f_1( x_1 w_1 + x_2 w_2 + b_1 ) w_3 + b_2 )$$

$$y = f_2( f_1( W X + B_1 ) w_3 + B_2 )$$

$$W = [w_1, w_2], X = [x_1; x_2]$$

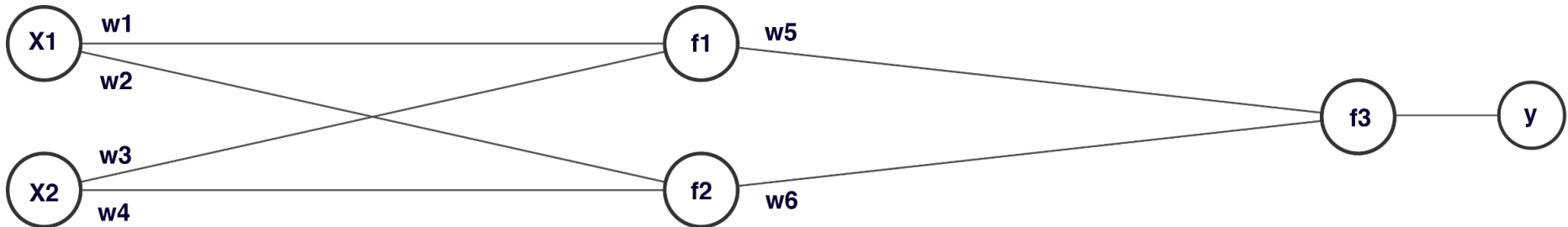


# Neural Network – example2

$$y = f_3(f_1(x_1w_1 + x_2w_2 + b_1)w_5 + f_1(x_1w_3 + x_2w_4 + b_2)w_6 + b_3)$$

$$y = f_3(f_1(X_1W_1 + B_1)w_5 + f_1(XW_2 + B_2)w_6 + B_3)$$

$$W_1[w_1, w_2], \quad X = [x_1; x_2], \quad W_2 = [w_3, w_4]$$

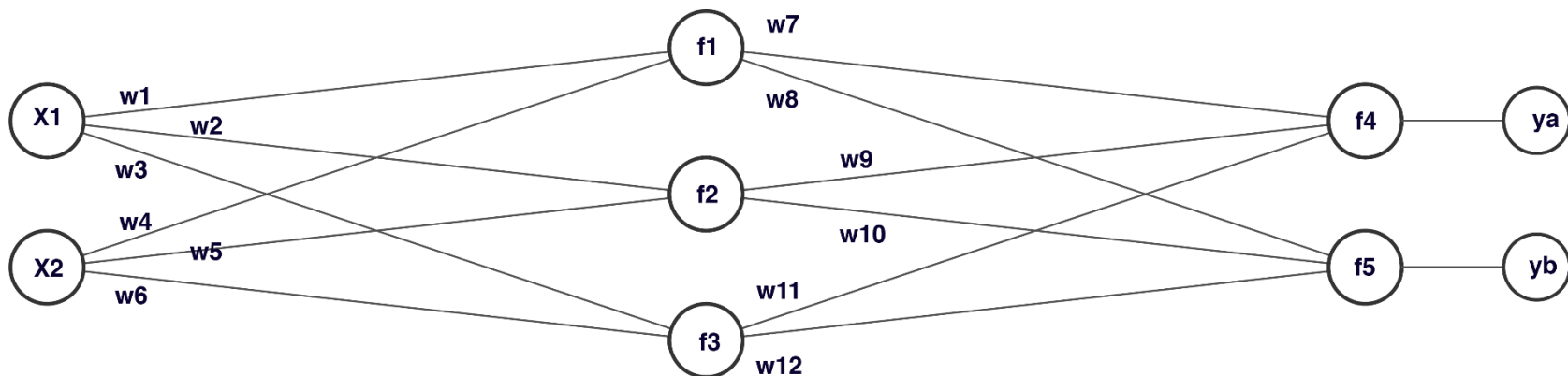


# Neural Network – example3

$$y_a = f_4 \left( \begin{array}{c} f_1(XW_1 + B_1)w_7 + f_2(XW_2 + B_2)w_9 + \\ f_3(XW_3 + B_3)w_{11} + B_4 \end{array} \right)$$

$$y_b = f_5 \left( \begin{array}{c} f_1(XW_1 + B_1)w_8 + f_2(XW_2 + B_2)w_{10} + \\ f_3(XW_3 + B_3)w_{12} + B_4 \end{array} \right)$$

$$X = [x_1, x_2], \quad W_1 = [w_1; w_4], \quad W_2 = [w_2; w_5], \quad W_3 = [w_3; w_6]$$



# Building blocks

---

- Software
- Building blocks
  - Neurons
  - **Loss functions**
  - Back propagation
- Practicalities
- Architectures
- Problems / questions

# Loss function

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- Compare output to wanted output (just error measurement)
- Mean Squared Error:  $(y_{pred} - y)^2$
- Cross Entropy:  $y \cdot \log(y_{pred})$
- Custom ones



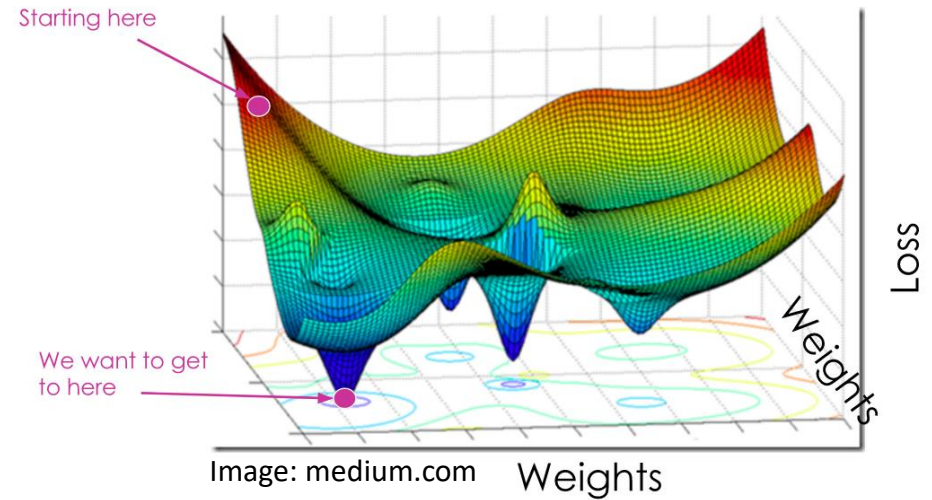
# Building blocks

---

- Software
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# Back propagation

- Relate loss to weights
- Differentiate loss on weights
  - Partial derivatives



# Recap: Differentiation

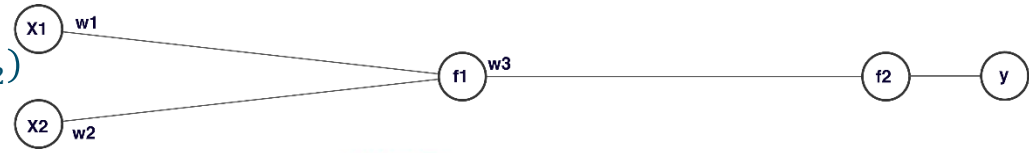
| Differentiation Rules |   |
|-----------------------|---|
| Constant Rule         | $\frac{d}{dx}[c] = 0$   |
| Power Rule            | $\frac{d}{dx}x^n = nx^{n-1}$  |
| Product Rule          | $\frac{d}{dx}[f(x)g(x)] = f'(x)g(x) + f(x)g'(x)$                                      |
| Quotient Rule         | $\frac{d}{dx}\left[\frac{f(x)}{g(x)}\right] = \frac{g(x)f'(x) - f(x)g'(x)}{[g(x)]^2}$ |
| Chain Rule            | $\frac{d}{dx}[f(g(x))] = f'(g(x))g'(x)$   |

$$\frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dv} \cdot \frac{dv}{dx}$$

$$\begin{aligned}f(x) &= (2x - 2)^2 \\f(x) &= g(u), \quad u = 2x - 2, \quad g(u) = u^2 \\ \frac{\partial f}{\partial x} &= \frac{\partial g}{\partial u} * \frac{\partial u}{\partial x} = 2u * 2 = 4(2x - 2)\end{aligned}$$

# Backpropagation - example

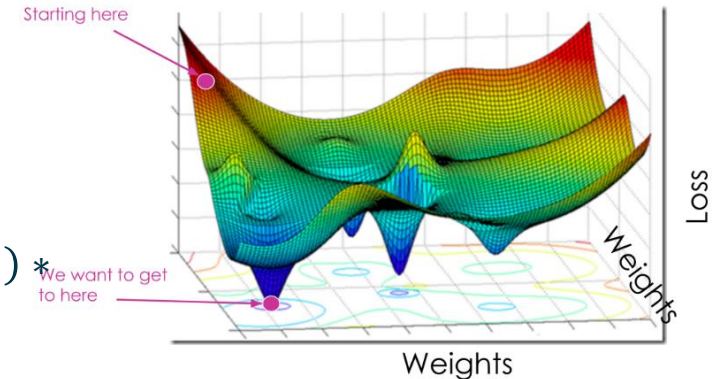
- $y_{pred} = f_2(f_1(x_1w_1 + x_2w_2 + b_1)w_3 + b_2)$
- $loss = (y - y_{pred})^2$



Remember  $f(x) = (2x - 2)^2$ ?

- $\frac{\partial Loss}{\partial w_1} = 2(f_1(f_1(XW + B_1)w_3 + B_2)) * -f'_2(f_1(XW + B_1)w_3 + B_2) * f'_2(XW + B_1)w_3 * x_1$
- $\frac{\partial Loss}{\partial w_2} = 2(f_1(f_1(XW + B_1)w_3 + B_2)) * -f'_2(f_1(XW + B_1)w_3 + B_2) * f'_2(XW + B_1)w_3 * x_2$
- $\frac{\partial Loss}{\partial w_3} = 2(f_1(XW + B_1)w_3 + B_2) * -f'_2(f_1(XW + B_1)w_3 + B_2) * f_1(XW + B_1)$

$$W = [w_1, w_2], \quad X = [x_1; x_2]$$



# Practicalities

---

- Software
- Building blocks
  - Neurons
  - Loss functions
  - Back propagation
- **Practicalities**
- Architectures
- Problems / questions

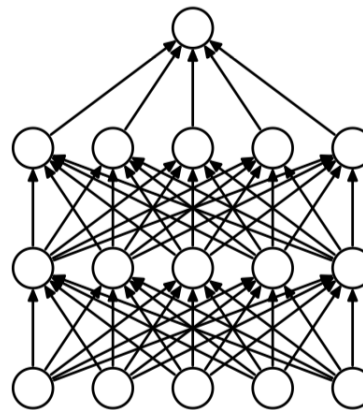
# Practicalities

- One hot encoding
- Dropout
- Batch normalization
- Padding

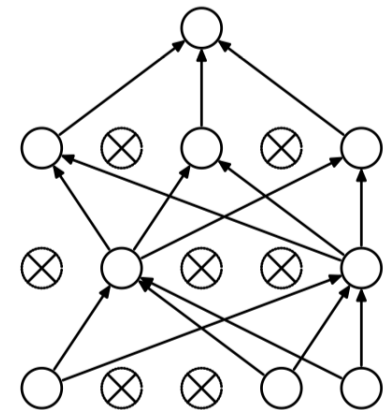
Rome = [1, 0, 0, 0, 0, 0, ..., 0]  
Paris = [0, 1, 0, 0, 0, 0, ..., 0]  
Italy = [0, 0, 1, 0, 0, 0, ..., 0]  
France = [0, 0, 0, 1, 0, 0, ..., 0]

word V

**ARLMP --> ARLMP**  
**ALP --> ALP \* \***  
**RNY Y --> RNY Y \***



(a) Standard Neural Net



(b) After applying dropout.

# Architectures

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- Software
- Building blocks
  - Neurons
  - Loss functions
  - Back propagation
- Practicalities
- **Architectures**
- Problems / questions

# Architectures

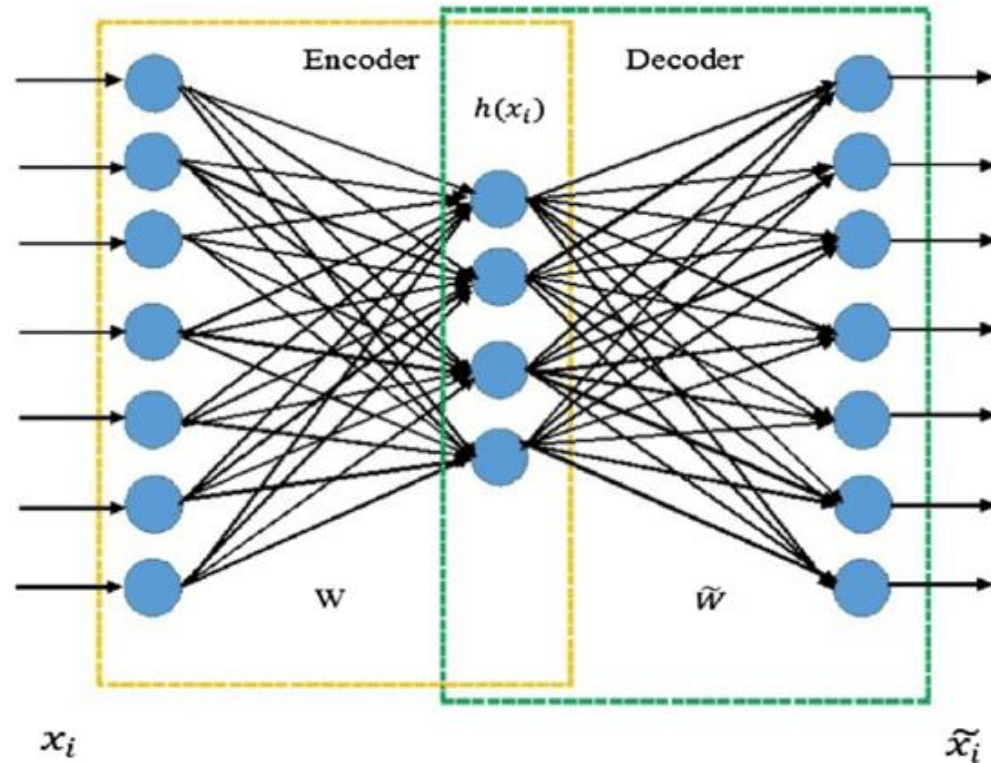
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- Fully Connected
- Auto encoder
- Recurrent Neural Network (RNN)
- Convolutional Neural Network (CNN)
- Generative Adversarial Network (GAN)



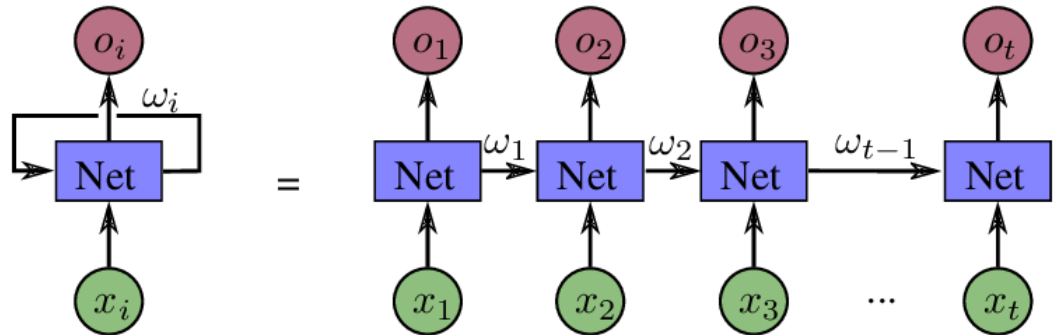
# Auto encoder

- Input = output
- Compress data



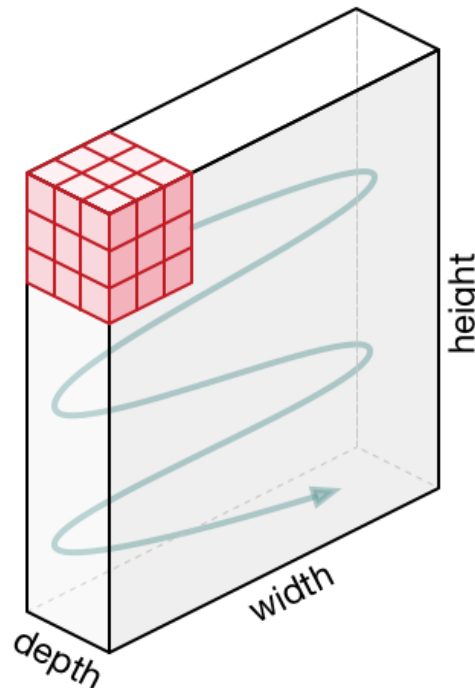
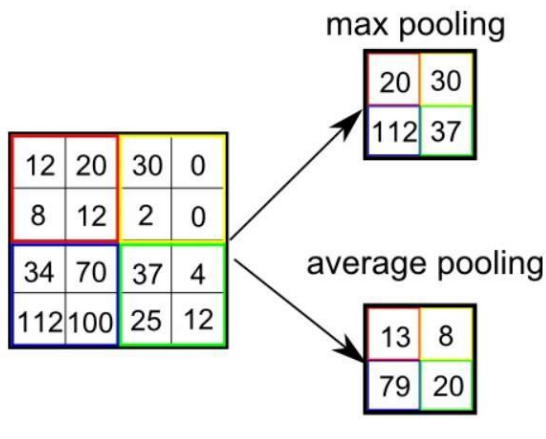
# Recurrent neural network

- Memory
- Variable input length
  - Same amount of features!
- Variable output length



# Convolutional neural network

- Windows
- Re-usable patterns
- Depth = amount of filters
- Pooling



|                 |                 |                 |   |   |
|-----------------|-----------------|-----------------|---|---|
| 1 <sub>x1</sub> | 1 <sub>x0</sub> | 1 <sub>x1</sub> | 0 | 0 |
| 0 <sub>x0</sub> | 1 <sub>x1</sub> | 1 <sub>x0</sub> | 1 | 0 |
| 0 <sub>x1</sub> | 0 <sub>x0</sub> | 1 <sub>x1</sub> | 1 | 1 |
| 0               | 0               | 1               | 1 | 0 |
| 0               | 1               | 1               | 0 | 0 |

Image

|   |  |  |
|---|--|--|
| 4 |  |  |
|   |  |  |
|   |  |  |

Convolved Feature

|                 |                 |                 |   |   |
|-----------------|-----------------|-----------------|---|---|
| 1 <sub>x1</sub> | 1 <sub>x0</sub> | 1 <sub>x1</sub> | 0 | 0 |
| 0 <sub>x0</sub> | 1 <sub>x1</sub> | 1 <sub>x0</sub> | 1 | 0 |
| 0 <sub>x1</sub> | 0 <sub>x0</sub> | 1 <sub>x1</sub> | 1 | 1 |
| 0               | 0               | 1               | 1 | 0 |
| 0               | 1               | 1               | 0 | 0 |

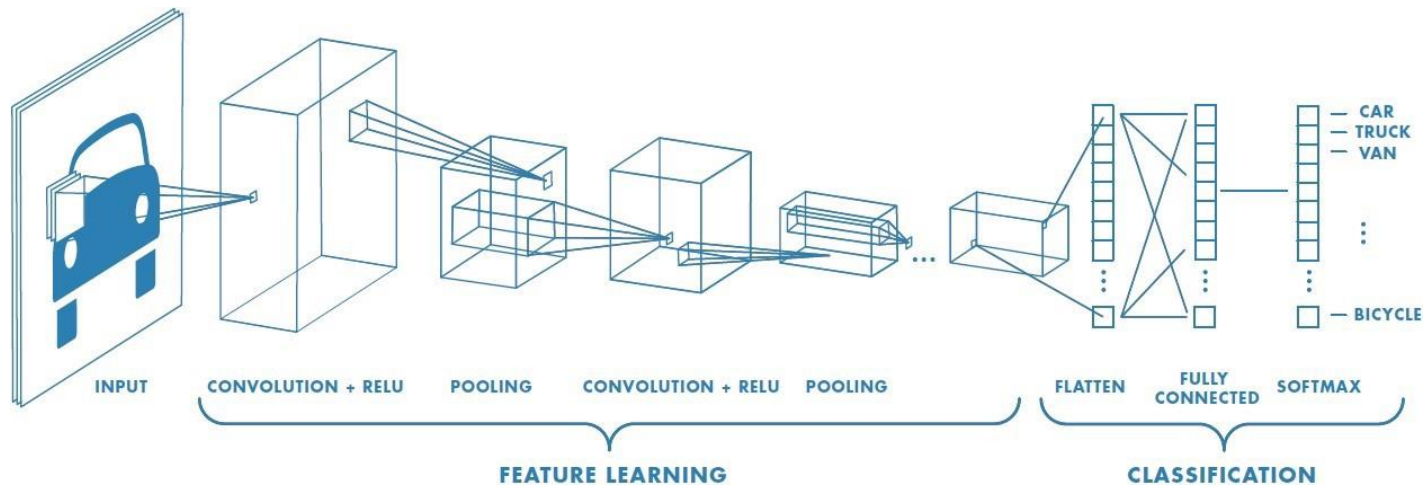
Image

|   |  |  |
|---|--|--|
| 4 |  |  |
|   |  |  |
|   |  |  |

Convolved Feature

# Convolutional neural network

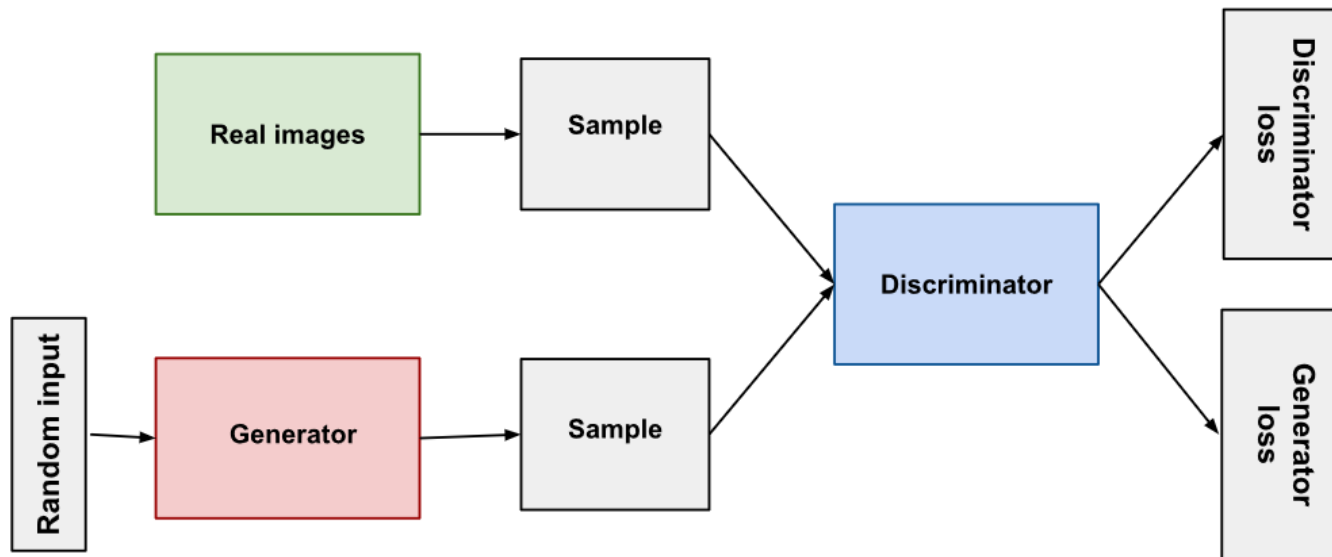
- Filters on filters
- New data representation



<https://towardsdatascience.com/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way-3bd2b1164a53>

# GANs

- Network vs network



# Problems / questions

---

- Software
- Building blocks
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  - Loss functions
  - Back propagation
- Practicalities
- Architectures
- **Problems / questions**

# Problems

---

- Get right input (represent features)
- Get good loss function (no problem vs youre welcome)
- Check output (no shortcuts? Overfitting?)
- Get good architecture
- **Need domain knowledge**

# Further reading

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## Links I used:

- <https://leonardoaraujosantos.gitbooks.io/artificial-inteligence/content/>
- <https://towardsdatascience.com/getting-started-with-pytorch-part-1-understanding-how-automatic-differentiation-works-5008282073ec>
- <https://www.digitalvidya.com/blog/types-of-neural-networks/>
- <https://blog.floydhub.com/long-short-term-memory-from-zero-to-hero-with-pytorch>
- <https://towardsdatascience.com/illustrated-guide-to-lstms-and-gru-s-a-step-by-step-explanation-44e9eb85bf21>
- <https://blog.floydhub.com/gru-with-pytorch/>
- <https://towardsdatascience.com/understanding-gru-networks-2ef37df6c9be>
- <https://medium.com/udacity-pytorch-challengers/a-brief-overview-of-loss-functions-in-pytorch-c0ddb78068f7>
- <https://playground.tensorflow.org/>

## Papers:

- “Convolutional Neural Network Architectures for Matching Natural Language Sentences”
- “Deep Visual-Semantic Alignments for Generating Image Descriptions”
- Papers by D.T. Rademaker



# Questions

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